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Resonances in positronium-rubidium and positronium-cesium scattering

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Abstract

Scattering of ortho positronium (Ps) by cesium and rubidium atoms has been investigated employing a three-Ps-state coupled-channel model with Ps(1s,2s,2p) states using a time-reversal-symmetric regularized electron-exchange model potential. We find a narrow S-wave singlet resonance at 5.057 eV of width 0.003 eV in the Ps-Rb system and at 5.067 eV of width 0.003 eV in the Ps-Cs system. Singlet P-wave resonances in both systems are found at 5.3 eV of width 0.4 eV. Singlet D-wave structures are found at 5.4 eV in both systems. The pronounced P- and D-wave resonances in these systems lead to easily detectable local minima in the low-energy elastic cross sections. We also report results for elastic and Ps-excitation cross sections for Ps scattering by Rb and Cs.

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Recent measurements of ortho positronium (Ps) scattering cross section by H_2, N_2, He, Ne, Ar, C_4H_{10}, and C_5H_{12} [1–7] have initiated new theoretical investigations [8–14] in this subject. We suggested [15–17] a regularized, symmetric, nonlocal electron-exchange model potential and used it in the study of Ps scattering by H [18], He [16,17,19], Ne [19], Ar [19], H_2 [20], Li [21], Na [22] and K [22]. The low-energy cross sections obtained in these studies are in agreement with experimental measurements for He [3,4] , Ne [7], Ar [7] and H_2 [3,4]. These investigations also produced correct results for resonance and binding energies for the S wave electronic singlet state of Ps-H [9–12,18] and Ps-Li [21] systems in addition to experimental pick-off quenching rate in Ps-He [17] scattering. These studies also predicted low-energy resonances in lower partial waves of the Ps-Na and Ps-K systems [22].

In this Letter we apply the above symmetric model-exchange potential to study Ps-Rb and Ps-Cs scattering using the three-Ps-state coupled-channel method. The interaction in the singlet channel is attractive in nature as in the corresponding channel of the Ps-H system [18] and we find resonances in this channel at low energies in S, P and D waves of both systems near the Ps(2) excitation threshold. We also report angle-integrated elastic and Ps-excitation cross sections for both systems.

The resonances in electron-atom [23–25] and positron-atom [26] systems, and in other atomic systems in general, are of great interest. Several resonances in the electron-hydrogen system have been found in the close-coupling calculation and later reconfirmed in the variational calculation [27–29]. Resonances have also been found in the close-coupling calculation of electron scattering by Li, Na and K [30,31]. These resonances provide the necessary testing ground for a theoretical formulation and can eventually be detected experimentally. A proper dynamical description of scattering in a theoretical formulation is necessary for the appearance of these resonances. The ability of the present exchange potential to reproduce the resonances in diverse Ps-atom systems [18,21,22] assures its realistic nature.

For target-elastic scattering we solve the following Lippmann-Schwinger scattering integral equation in momentum space [16,18]

$$f^{\pm}_{\nu',\nu}(\mathbf{k}',\mathbf{k}) = \mathcal{B}^{\pm}_{\nu',\nu}(\mathbf{k}',\mathbf{k}) - \sum_{\nu''} \int \frac{\mathrm{d}\mathbf{k}''}{2\pi^2} \frac{\mathcal{B}^{\pm}_{\nu',\nu''}(\mathbf{k}',\mathbf{k}'') f^{\pm}_{\nu'',\nu}(\mathbf{k}'',\mathbf{k})}{k^2_{\nu''}/4 - k''^2/4 + \mathrm{i}0}, \tag{1}$$

where the singlet (+) and triplet (−) "Born" amplitudes, $\mathcal{B}^{\pm}$, are given by $\mathcal{B}^{\pm}_{\nu',\nu}(\mathbf{k}',\mathbf{k}) = g^D_{\nu',\nu}(\mathbf{k}',\mathbf{k}) \pm g^E_{\nu',\nu}(\mathbf{k}',\mathbf{k})$, where g^D and g^E represent the direct and exchange Born amplitudes

and the $f^{\pm}$ are the singlet and triplet scattering amplitudes, respectively. The quantum states are labeled by the indices ν, referring to the Ps atom. The variables $\mathbf{k}$, $\mathbf{k}'$, $\mathbf{k}''$ etc denote the appropriate momentum states of Ps; $\mathbf{k}_{\nu''}$ is the on-shell relative momentum of Ps in the channel ν''. We use units $\hbar = m = 1$ where m is the electron mass.

To avoid the complication of calculating exchange potential with a many-electron wave function, we consider a frozen-core one-valence-electron approximation for the targets Rb and Cs. Such wave functions have been successfully used for scattering of alkali metal atoms in other contexts and also for positronium scattering by Li [13,14]. The Rb(5s) and Cs(6s) frozen-core hydrogen-atom-like wave functions are taken as

$$\phi_{\rm Rb}(\mathbf{r}) = \frac{1}{300\sqrt{5}\sqrt{4\pi\bar{a}_0^3}}(120 - 240\rho + 120\rho^2 - 20\rho^3 + \rho^4)e^{-\rho/2}, \tag{2}$$

$$\phi_{\rm Cs}(\mathbf{r}) = \frac{1}{2160\sqrt{6}\sqrt{4\pi\bar{a}_0^3}}(720 - 1800\rho + 1200\rho^2 - 300\rho^3 + 30\rho^4 - \rho^5)e^{-\rho/2}, \tag{3}$$

where $\rho = 2r\alpha$ with $\alpha = 1/(n\bar{a}_0)$. Here $n = 5$ for Rb and $= 6$ for Cs and $\bar{a}_0 = (2n^2E_i)^{-1}a_0$ with E_i the ionization energy of the target in atomic unit and a_0 the Bohr radius of H. Here we use the following experimental values for ionization energies for Rb and Cs, respectively: 4.176 eV and 3.893 eV [32].

In this coupled-channel calculation we employ the above frozen-core approximation for the target wave function. In addition we shall neglect the excited states of the target and employ only the lowest Ps(2) excitations of the Ps. Although, such an approximation is not entirely realistic, specially when these excitations are energetically open, it makes this complicated scattering process mathematically tractable. Moreover, previous experience with Ps-Li, Ps-Na, and Ps-K systems in similar three-Ps-state model has revealed interesting physics in producing resonances and correct binding energies [21,22]. The reproduction of correct binding energies assures of physically plausible low-energy cross sections. Hence we believe that the present study of Ps-Rb and Ps-Cs scattering should lead to physically reasonable results. However, it would be interesting to repeat this investigation in the future including the excited states of the target, as has been by Ray in the Ps-Li system [14], as well as of Ps, and compare the results for low-energy scattering with the present investigation.

The direct Born amplitude of Ps scattering is given by [16]

$$g^D_{\nu',\nu}(\mathbf{k_f}, \mathbf{k_i}) = \frac{4}{Q^2}\int \phi^*(\mathbf{r})\left[1 - \exp(\mathrm{i}\mathbf{Q}.\mathbf{r})\right]\phi(\mathbf{r})\mathrm{d}\mathbf{r}$$

$$\times \int \chi^*_{\nu'}(\mathbf{t}) 2\mathrm{i} \sin(\mathbf{Q}.\mathbf{t}/2) \chi_\nu(\mathbf{t}) \mathrm{d}\mathbf{t}, \tag{4}$$

where $\phi(\mathbf{r})$ is the target wave function and $\chi(\mathbf{t})$ is the Ps wave function. The (parameter-free) exchange amplitude corresponding to the model potential is given by [18]

$$g^E_{\nu',\nu}(\mathbf{k_f}, \mathbf{k_i}) = \frac{4(-1)^{l+l'}}{D} \int \phi^*(\mathbf{r}) \exp(\mathrm{i}\mathbf{Q}.\mathbf{r}) \phi(\mathbf{r}) \mathrm{d}\mathbf{r}$$
$$\times \int \chi^*_{\nu'}(\mathbf{t}) \exp(\mathrm{i}\mathbf{Q}.\mathbf{t}/2) \chi_\nu(\mathbf{t}) \mathrm{d}\mathbf{t}, \tag{5}$$

with $D = (k_i^2 + k_f^2)/8 + \alpha^2 + (\beta_\nu^2 + \beta_{\nu'}^2)/2$ where l and l' are the angular momenta of the initial and final Ps states. The initial and final Ps momenta are $\mathbf{k_i}$ and $\mathbf{k_f}$, $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f}$, and β_ν^2 and $\beta_{\nu'}^2$ are the binding energies of the initial and final states of Ps in atomic unit, respectively. The exchange potential for Ps scattering is considered [15] to be a generalization of the Ochkur-Rudge exchange potential for electron scattering [33,34]. It is possible to introduce an adjustable parameter in the above exchange potential to fit the scattering result to an accurately known low-energy observable, such as the Ps-atom scattering length or binding energy [19]. However, in Ps-Rb and Ps-Cs systems there is no such observable and we use the parameter-free exchange amplitude (5) in this investigation.

After a partial-wave projection, the system of coupled equations (1) is solved by the method of matrix inversion. Forty Gauss-Legendre quadrature points are used in the discretization of each momentum-space integral. The calculation is performed with the exact Ps wave functions and frozen-core orbitals (2) and (3) for Rb(5s) and Cs(6s) ground state. We consider Ps-Rb and Ps-Cs scattering using the three-Ps-state model that includes the following states: Ps(1s)Rb(5s), Ps(2s)Rb(5s), Ps(2p)Rb(5s), and Ps(1s)Cs(6s), Ps(2s)Cs(6s), Ps(2p)Cs(6s), for Rb and Cs, respectively.

The Ps-Rb and Ps-Cs systems have an effective attractive interaction in the singlet channel as in the Ps-H [18] and Ps-Li [21] systems. The targets of these systems have one active valence electron outside a closed shell. In the coupled-channel calculation we find resonances in both systems in the singlet state. No resonances appear in the triplet state. For the resonances to appear, the inclusion of the excited states of Ps is fundamental in a coupled-channel calculation. The static-exchange model with both the target and Ps in the ground state does not lead to these resonances. A detailed investigation of these resonances in coupled-channel model of Ps-H [9–11,18] and Ps-Li [21] systems in the singlet state has appeared in the literature.

Here to study the resonances, first we calculate the S-, P- and D-wave elastic phase shifts and cross sections in the singlet channel of the Ps-Rb and Ps-Cs systems using the 3-Ps-state model. The phase shifts are calculated in the usual fashion [35] from the partial-wave scattering amplitude or from the partial-wave S matrix. The energy and width of resonance are obtained by fitting the corresponding partial-wave cross section to the well-known Breit-Wigner formula

$$\sigma(E) \sim \frac{\pi}{k^2} \frac{\Gamma^2}{(E - E_R)^2 + \Gamma^2/4}, \tag{6}$$

where $\sigma(E)$ is the cross section at energy $E = 6.8k^2$ eV, E_R is the resonance energy and Γ the width. The S-wave phase shifts are shown in Fig. 1. The Ps-Rb system has a resonance at 5.057 eV of width 0.003 eV. The resonance in the Ps-Cs system appears at 5.067 eV and also has a width 0.003 eV. The phase shift curves in Fig. 1 clearly show the resonances where the phase shifts jump by π.

In Fig. 2 we show the P-wave Ps-Rb and Ps-Cs phase shifts in the singlet state. Both systems possess resonances at 5.2 eV of width of 0.3 eV. The P-wave singlet elastic cross section at low energies shown in the off-set clearly exhibits these resonances. In Fig. 3 we plot the D-wave singlet elastic cross section for Ps-Rb and Ps-Cs systems at low energies. There is a structure in both systems at 5.4 eV which is more diffuse than in S and P waves.

Next we calculate the different partial cross sections of Ps-Rb and Ps-Cs scattering. The convergence of the cross sections with respect to partial waves is slower in this case than in the case of Ps-H scattering. At a incident Ps energy of 50 eV, 40 partial waves were used to achieve convergence of the partial-wave scheme. In Figs. 4 and 5 we plot different angle-integrated cross sections of Ps-Rb and Ps-Cs scattering, respectively. Specifically, we plot the elastic, Ps(2s) and Ps(2p) excitation cross sections using the three-Ps-state model. For comparison we also plot the elastic cross section obtained with the static-exchange model. The elastic cross section is large at low energies in both systems. In the off-set of Figs. 4 and 5 we plot the corresponding low-energy elastic cross sections. The effect of the inclusion of highly polarizable Ps(2) states in the coupling scheme could be considerable, specially at low energies.

From Figs. 4 and 5 we see that the P and D-wave resonances of large widths predicted in this Letter have lead to local minima in the elastic cross section below the Ps excitation threshold at 5.1 eV. Hence these resonances can be easily detected experimentally after an

analysis of the elastic scattering cross section at low energies. This makes these resonances of great experimental interest. Similar minima appear in the cross section for electron scattering by alkali-metal atoms due to appearance of resonances in these systems [19,31]. However, the S-wave resonances in the Ps-Rb and Ps-Cs systems are narrow and may not be easily noted experimentally from a simple analysis of the cross sections.

To summarize, we have performed a three-Ps-state coupled-channel calculation of Ps-Rb and Ps-Cs scattering at low energies using a regularized symmetric nonlocal electron-exchange model potential [15,16] successfully used [16,18–21] previously in different Ps scattering problems. We present the results of angle-integrated partial cross sections at different Ps energies. We also present results for singlet phase shifts and partial-wave cross sections at low energies to study the resonances in these systems. We find resonances in S, P and D waves near the Ps(2) excitation threshold. In this Letter we have used a three-Ps-state model. Similar resonances have been found in the coupled-channel model of electron-H [27–29], electron-Na, electron-K [30,31], positron-hydrogen [26], Ps-H [10,11,18] and Ps-Li [21] systems. In most cases, a more complete calculation and (in some cases) experiments have reconfirmed these resonances. In view of this we do not believe that the appearance of these resonances in the present three-state calculation to be so peculiar as to have no general validity. However, the resonance energies might change slightly after a more complete calculation as in electron-H, positron-H and Ps-H systems and it would be intersting to study the present resonances using more complete theoretical models in the future in addition to compare the present results with future experiments.

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Figure Caption:

1. Singlet S-wave elastic phase shift at different Ps energies for Ps-Rb (dashed line) and Ps-Cs (full line) scattering.

2. Singlet P-wave elastic phase shift at different Ps energies for Ps-Rb (dashed line) and Ps-Cs (full line) scattering. The corresponding P-wave singlet cross section is shown in the off-set.

3. Singlet D-wave elastic cross section at different Ps energies for Ps-Rb (dashed line) and Ps-Cs (full line) scattering.

4. Partial cross sections for Ps-Rb scattering at different Ps energies: three-Ps-state elastic (full line), three-Ps-state Ps(2s) (dashed-dotted line), three-Ps-state Ps(2p) (short-dashed line), static-exchange elastic (long-dashed line). Three-Ps-state (full line) and static-exchange (long-dashed line) elastic results at low energies are also shown in the off-set.

5. Same as in Fig. 4 for Ps-Cs scattering.